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Enhancements to the Atmospheric Transmittance/Radiance Program FASCODE

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OptiMetrics, Inc. 121 Middlesex Turnpike Burlington, MA 01803

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This report describes software enhancements to the atmospheric transmittance/radiance program FASCODE which allows the user to easily and directly compare FASCODE calculations with measured spectra. The enhancements include						
the capability to: a. Convert a file containing a measured spectrum into the format of a FASCODE calculation,						
b. Interpolate a spectrum in a FASCODE format onto an arbitrary frequency grid,						
c. Take the point-by-po the same frequency g	rid, and					
d. Plot the individual spectra and their difference on the same graph.						
Also included in the report are FASCODE calculations of transmittance versus range for a sensor operating at 30 km such as SCRIBE (Stratospheric Cryogenic_						
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Laurence Rothman		<u>l</u>		_1	AFCL /OPI	

Interferometer Balloon Experiment.) These calculations should aide interpreting the data from SCRIBE by indicating which region of the atmosphere the emission at different wavenumbers comes from.

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1. INTRODUCTION

FASCODE¹ is a model and a computer program for computing atmospheric transmittance and radiance using the line-by-line method. **FASCODE** has become the industry standard for such calculations because of its power and flexibility, its wide distribution and its ongoing support. One common use of **FASCODE** is to simulate atmospheric measurements of transmittance or radiance². The comparison between the measurements and the calculations can be used for example, to improve the model or to detect new molecules in the atmosphere.

Up to now, the comparison between the calculated and the measured spectra has been limited to plotting them on the same graph and visually inspecting the result. In order to improve the capabilities of **FASCODE** in this area, several computer programs were created which allow the user to take and plot the point-by-point difference between spectra. These programs can:

- a. Convert a file containing a measured spectrum into the format of a FASCODE calculation,
- b. Interpolate a spectrum in a **FASCODE** format onto an arbitrary frequency grid,

^{1.} Clough, S. A., F. X. Kneizys, E. P. Shettle, and G. P. Anderson (1986) Atmospheric Radiance and Transmittance: FASCODE 2, in the Sixth Conference on Atmospheric Radiation, Williamsburg, Virginia, May 13-16, 1986

Dowling, J. A., W. O. Gallery and S. G. O'Brien (1984), Analysis of Atmospheric Interferometer Data, Air Force Geophysics Laboratory, Hanscom AFB, Massachusetts, AFGL-TR-84-0177, ADA150682

- c. Take the point-by-point difference between two FASCODE format files with the same frequency grid, and
- d. Plot the individual spectra and their difference on the same graph.

These capabilities will be demonstrated with examples of comparisons between **FASCODE** calculations and measurements from the SCRIBE experiment³.

As an aid in interpreting the data from SCRIBE, several types of calculations were made using **FASCODE**. The object of these calculations is to determine the origin of the radiance in the opaque region around 667 cm^{-1} and in the window region between $800 \text{ and } 820 \text{ cm}^{-1}$. These calculations include calculations of transmittance versus wavenumber for various ranges in the 667 cm^{-1} region and for contour plots of constant transmittance on an altitude versus wavenumber plot in both the 667 cm^{-1} and the $800-820 \text{ cm}^{-1}$ regions.

^{3.} Gallery, W. O., D. Longtin, and G. Tucker (1987), SCRIBE Data Survey and Analysis, Air Force Geophysics Laboratory, Hanscom AFB, Massachusetts, AFGL-TR-87-0061. (ADA183538)

2. FASCODE ENHANCEMENTS

Three computer programs were created to enhance the ability of users to compare measured spectra with FASCODE calculations. The programs and their functions are:

FSCFMT Converts a file containing a measured spectrum into a file with the format of a FASCODE calculation.

INTDIF Interpolates a FASCODE format file onto a specified wavenumber grid and takes the point-by-point difference between two FASCODE format files.

FSCPLOT Plots one or more spectra in FASCODE format on the same graph with options for plotting colors, symbols and dashed lines plus for scaling the plotted values*.

These three programs will be discussed separately in the next sections. The user's guides for the three programs are in Section 3. A listing of the programs is not included here, but the source code is available from AFGL/OPI on tape or on 5.25 inch floppy disk.

2.1 FSCFMT

FSCFMT takes a measured spectrum and puts it into the format of a FASCODE file. This "pseudo-FASCODE" file may then be manipulated by FASCODE; for example, it can be plotted, degraded with an instrument function, or have a filter function passed over it. It may also be manipulated by the programs INTDIF and FSCPLOT.

^{*} FSCPLOT was originally developed by W. Gallery while employed at AFGL. However the version presented here has been improved and enhanced and documented for the first time.

The format of a FASCODE file is a binary file with four different kinds of records. The first record of a file is a header record which contains identifying information on the FASCODE run which produced the file and has various flags indicating what kind of data are in the file. The identifying information includes: a user supplied title, the date and time of the run, the version of FASCODE, used the atmospheric conditions (number of layers, average pressure and temperature and total absorber amounts for the gases included), initial and final wavenumber and wavenumber increment and the shape and width of the scanning function used (if any). The flags indicate whether the file contains transmittance, radiance, or radiance and transmittance, and whether the data are monochromatic or has been degraded with a scanning function.

The spectral data are written in records of up to 2400 words each and are called panels. Each panel is preceded by a panel header of four words giving the initial and final wavenumber of the following panel, the wavenumber increment and the number of points. The panel/header-panel combination is clearly repeated until the end of the spectrum. The end of the data is indicated by a record of six words, in length all equal to integer -99. Multiple FASCODE spectra may be included on a single file by following the end-of-data record with the header record of the next spectrum.

FSCFMT writes the measured spectrum into a file with the FASCODE format with the following differences. The

PASCODE version is replaced by the word "MEASURED" and the user supplies values for the other identifying information.

Also, since all measurements have a finite resolution, the flags are set to indicate that the data have been degraded with an instrument function.

FSCFMT is set up to read spectral data from an ASCII file in a particular format but can easily be modified to accommodate any other format. The measured spectrum is read in the subroutine MANIP. The appropriate READ and FORMAT statements are indicated in comment statements.

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2.2 INTDIF

To compare two spectra point-by-point, the spectra need to be defined on the same wavenumber grid. The program INTDIF interpolates the spectrum contained on a FASCODE format file onto the same wavenumber grid as that of a second FASCODE format file using linear interpolation between adjacent points. The program next writes the point-by-point difference between the two to a third FASCODE format file which can then be plotted.

When using INTDIF, the following points should be kept in mind.

- a. It is better to interpolate the calculated spectrum rather than the measured spectrum because the calculated spectrum is typically on a finer grid (oversampled) than the measurement so there is less interpolation error. Also, a measurement always contains noise and it is better not to interpolate noise.
- b. The user specifies separately the differencing and the interpolation range. The interpolation range should be set at least slightly smaller than the

range of the calculation to avoid possible problems interpolating at the endpoints.

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- c. INTDIF writes the interpolated spectrum to the file TAPEll and the differenced spectrum to TAPEl2. Both files are in the form of FASCODE format files.
- d. INTDIF can only take the difference between files of the same type, e.g. both containing radiance or both transmittance. It cannot difference files where one contains optical depth (e.g. a monochromatic transmittance calculation), and the other transmittance (a measurement file from FSCFMT or a degraded calculation).

2.3 FSCPLOT

FASCODE format files. The improvements over the standard FASCODE plotting package are:

- a. Multiple curves can be plotted on the same grid.
- b. The curves can be drawn with or without symbols, in four different colors, or as dashed lines.
- c. Both the frequency and the Y axis values may be scaled before plotting.

With FSCPLOT, a measurement, a calculation and their difference can all be shown on the same graph. Also, the difference can be enlarged and offset to better display small details. In certain cases, FSCPLOT must convert the data on the file to the units on the Y axis, e.g. from to transmittance or from radiance to optical depth brightness temperature. The Y axis values may be scaled linearly with user supplied parameters either before or after conversion. The frequency values may be scaled quadratically. This option is designed specifically to

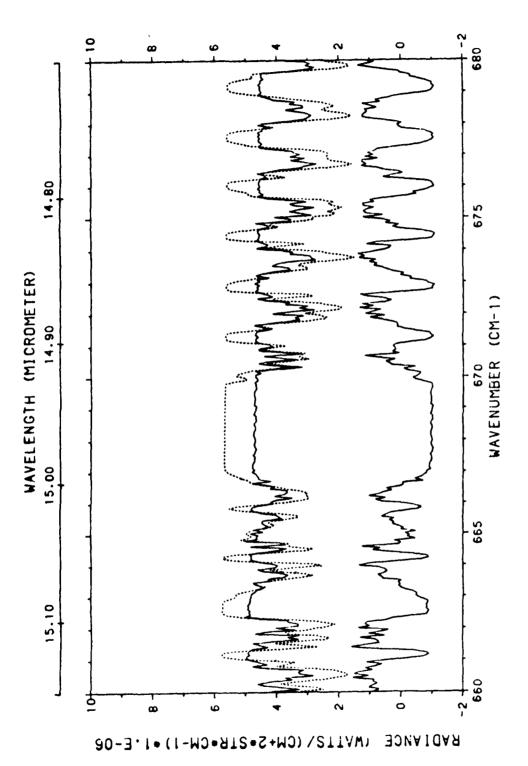
adjust the wavenumber scale of diode laser measurements which have not been properly been calibrated with an etalon. **FSCPLOT** is set up to run as a separate program but it may be substituted for the plot package in FASCODE itself. All the plots shown here were produced by FSCPLOT.

2.4 Examples

This section shows a plot resulting from the use of the programs FSCFMT, INTDIF and FSCPLOT. The measured data is from the SCRIBE experiment which is a balloon borne fourier transform spectrometer measuring infrared emission from the atmosphere. The data from this experiment are being validated and analyzed in a separate study*.

Figure 1 shows part of a measured spectrum from the SCRIBE experiment (solid line) compared with a FASCODE calculation (dashed line) and the difference between the two (bottom curve). The spectrum is from the July 5, 1984 flight and was obtained by co-adding 8 individual spectra*. The sensor was at the float altitude of 30.5 km looking slightly above the horizontal with a zenith angle of 88.1 deg. The FASCODE calculation used a companion radiosonde profile extrapolated to 45 km using the US Standard Atmosphere 1976. The calculated radiance was degraded with a triangular instrument function with a half width at half

^{*} This spectrum was provided by Aaron Goldman, Dept. of Physics, University of Denver.



and Difference gle of 88.1 a Zenith Angle of Measured Spectrum SCRIBE 84-1 (solid line) Between 660 cmversus FASCODE Calculation (dashed line) and Their Differve). The Sensor is at 30 km Looking at a Zenith Angle of (bottom curve). Figure_{.680 cm_

4444440P222332340B39222240B3334

In the figure, the broad flat feature between 667 and 670 cm $^{-1}$ is the Q branch of the e₃ band of CO₂, the peaks on both sides are the P and R branch lines. The comparison between the measurement and the calculation shows a systematic difference of about 1.0 watt/(cm² ster cm⁻¹) at the peaks of all the lines. In the valleys between the lines, the calculations go much deeper than the measurements indicating that the calculated transmittance out to space is less than the actual. Between the lines where the radiance is changing rapidly, the difference spectrum shows more clearly the presence of a sharp feature found in spectrum but not the other. For example, at 670.6 cm⁻¹ there is a feature in the measurement not seen calculation. This difference shows more clearly in differenced spectrum than in the clutter of the two original spectra.

3. USERS GUIDES FOR THE PROGRAMS FSCFMT, INTDIF, AND FSCPLT 3.1 FSCFMT

spectrum into a file in the FASCODE format. This file can then be manipulated as if it were a FASCODE calculation. In particular it can be plotted, degraded with an instrument function, have a filter passed over it, or be differenced with another FASCODE format file by the program INTDIF. The measured spectrum can be either transmittance or radiance. FSCFMT sets the appropriate flags in the file header to identify it to FASCODE. The user supplies identifying information for the title, time and date of the measurement, and the instrument function half width at half maximum. The program may be run in a batch mode or interactively, in which case the user is prompted for the input.

I/O Assignments:

Unit 5: User inputs (described later).

Unit 6: Standard output.

Unit 11: Input file containing measured spectrum.

Unit 12: Output file in FASCODE format.

User Inputs:

Card 1:

XID (A64): Title of measurement (64 characters max)

Card 2: HDATE, HTIME (A8,2X,A8)

HDATE: Date of measurement (YY/MM/DD).

HTIME: Time of measurement (HH:MM:SS).

Card 3: IEMIT (15)

IEMIT: Measurement is transmittance (0) or

radiance (1)

Card 4: HWHM (F10.3)

HWHM: Half width at half maximum of the instrument

function (cm⁻¹), assumed to be a triangle

(for information only).

Card 5: IDEBUG (15)

IDEBUG: Flag for printing debugging information on

unit 6(0 = no, $1 \approx yes$).

Input File Format:

The input data on unit ll should have the following format:

Line 1: IDY, DV, V1C (11X, I5, 26X, 2E18.11)

IDY: Total number of data points to follow.

DV: Wavenumber increment between points.

V1C: Starting wavenumber.

Line 2: DATA(I) (8E12.6)

DATA: The data, transmittance or radiance.

Line 2 is repeated until all IDY points are read in.

Program Notes:

The input file format is defined in subroutine MANIP where it is set off by comments. The user may easily change this format to suit any particular need. However, the data points are assumed to be equally spaced in wavenumber so that unequally spaced data (e.g. from a grating spectrometer or an uncalibrated diode laser) would have to be first interoplated onto an equally spaced grid.

3.2 INTDIF

INTDIF interpolates a spectrum on a FASCODE format file onto a user specified wavenumber grid and takes the point-by-point difference between the interpolated file and another FASCODE file. The program is typically used to compare a a FASCODE model calculation with a measurement which has been formatted with the program FSCFMT.

I/O Assignments:

Unit 5: User inputs.

Unit 6: Standard output.

Unit 11: Interpolated file, prior to differencing.

Unit 12: Input file #1, spectrum to be interpolated.

Unit 21: Differenced file, input file #2 minus

file #1.

Unit 22: Input file #2, spectrum to be differenced.

User Inputs:

Card 1: VII, V2I, DV

VII: Starting wavenumber for interpolation.

V2I: Ending wavenumber for interpolation.

DV: Wavenumber increment for the interpolated file. If DV = 0, then the value of DV from TAPE22 is used. If DV is not zero, then the

program stops after interpolating.

Card 2: VlD, V2D

VID: Starting wavenumber for differencing.

V2D: Ending wavenumber for differencing.

Program Notes:

Both of the input files must be in the FASCODE format and both must be of the same type, either both scanned transmittance or both scanned radiance. The program will not handle monochromatic (unscanned) data.

Input file #1 should be the FASCODE calculation and file #2 the measurement (the calculation typically has a finer spacing so there is less interpolation error and the measured spectrum contains noise).

User input is format free form, that is, without format control.

VII (V2I) should be larger (smaller) than the starting (ending) wavenumber VIC (V2C) of input file #1. If not, it is reset to V1C+DV (V2C-DV) to avoid potential problems interpolating at the endpoints.

Very rapidly changing data (e.g. narrow features) may cause erroneous points because of limits of the resolution of INTDIF.

The differenced data on unit 21 may contain negative values which will present problems if plotted on a log scale.

After interpolating, TAPEll is rewound and read and selected information is dumped. The fileheader is listed, and the wavenumber limits, the number of points and the first and last two points of each panel are printed. TAPEl2 is dumped in a similar manner after differencing.

3.3 FSCPLOT

FSCPLOT is an alternate package for plotting FASCODE format files. It can plot multiple curves on the same graph, draw curves in four colors and with symbols and/or dashed lines plus it can scale both the wavenumber values and the Y axis values before plotting them.

I/O Assignments:

Unit 5: User input.

Unit 6: Standard output.

Unit n: File "TAPEn" where n can be any number

less than 99 except 5, 6, or 39 (39 is reserved at AFGL for the plot file).

User Inputs:

Card 1: XID (A64)

> Run identification (64 characters max). XID:

Card 2: IPLOT (35X, 15)

> IPLOT: Enter a 1.

PLTID3 (A30) Card 3:

> PLTID3: Plot identification, printed on banner (30

> > characters max).

Card 4:

V1, V2, XSIZ, DELV, NUMSBX, NOENDX, IXDEC, IHEAD, SCALE

(4F10.3, 4I5, F10.3)

V1: Initial wavenumber of the X axis.

V2: Final wavenumber of the X axis.

Length of the X axis, in inches. XSIZ:

Number of wavenumbers per major division. DELV:

NUMSBX: Number of minor divisions per major division, e.g. DELV = 5 gives 4 small tick marks (5 compartments) per major division.

NOENDX: Control for the labels at the ends of the axis: O leaves both labels, I supresses the numbers at both ends, 2 supresses only the beginning label, and 3 supresses only the last label.

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IXDEC: Number of figures after the decimal point on the X axis; O gives no decimal point.

IHEAD: Control for the writing a plot header with file identification before each plot:

= 0: write header. = 1: no header.

SCALE: Scale factor for plot: scales the entire plot including the size of letters (default =1.0).

Card 5: YMIN, YMAX, YSIZ, DELY, NUMSBY, NOENDY, IYDEC, JEMIT, JPLOT, LOGPLT

(4F10.7, 6I5)

YMIN: Minimum value for the Y axis.

YMAX: Maximum value for the Y axis. If a log plot is selected, YMIN and YMAX are exponents.

YSIZ: Length of the Y axis, in inches.

DELY: Number of units of Y per major division. Ignored for a log plot.

NUMSBY: Number of minor divisions per major division. (see NUMSBX)

NOENDY: Controls the labels at the ends of the X axis. (see NOENDX)

IYDEC: Number of figures after the decimal point. (ignored for a log plot)

JEMIT: = 0 for plotting transmittance or optical depth.

= 1 for plotting radiance or brightness temperature.

JPLOT: For JEMIT = 0:

= 0: Y axis is transmittance.
= 1: Y axis is optical depth.

For JEMIT = 1:

= 0: Y axis is radiance. (Watts/(cm² ster cm¹).

= 1: Y axis is brightness temperature.
 (degrees Kelvin) (for YMAX greater
 than 1, see Program Notes).

LOGPLT: = 0 For linear Y axis. = 1 For log Y axis.

Card 6: LUNIT, LFILE, L4PT, LPEN, LDASH, LSYMBL, LSCALE (715)

LUNIT: > 0: Unit number of the file to be plotted. = 0: Finish this graph and read in Card 4 for the next graph.

< 0: Finish with plotting.

LFILE: Sequential number of the spectrum on LUNIT to be plotted. If LFILE = 0, plot the first spectrum.

L4PT: = 0: No interpolation.

= 1: Interpolate and plot three points between the given data points using Legrange 4 point interpolation.

LPEN: = 0: Default color.

= 1: Green. = 2: Black. = 3: Red. = 4: Blue.

LDASH: = 0: Draw a solid line. = 1: Draw a dashed line.

LSYMBL: > 0: Draw a symbol at each point and a line between points.

= 0: Draw only a line between points.< 0: Draw only a symbol at each point.

and 6b).

Cards 6a: YSCALE, YOFSET, YFAC, YDISPL (4F10.3)

YSCALE: Multiplicative factor for Y axis values,

applied before conversion (default = 1).

YOFSET: Additive factor for Y axis values, applied

befor conversion.

YFAC: Multiplicative factor for Y axis values,

applied after conversion (default = 1).

YDISPL: Additive factor for Y axis values, applied

after conversion.

Card 6b: XOFSET, XSCALE, XQUAD

XOFSET: Wavenumber offset.

XSCALE: Wavenumber scale factor (default = 1).

XQUAD: Wavenumber quadratic factor.

Program Notes:

The IHEAD = 1 option supresses the plot header and positions the left edge of the plot 2 inches from the left origin. This option is useful for plotting to a screen.

When plotting brightness temperature (JEMIT = 1 and JPLOT = 1) and YMAX is greater than 1.0, YMAX and YMIN are interpreted as temperatures, not as radiance values.

If LUINT is 0, the current graph is finished, and the program expects to find a new Card 4 starting a new graph. If LUNIT is negative, the program terminates.

Multiple spectra can be written to the same file. For example, the same spectrum can be scanned with different instrument functions and the results all written to the same file. LFILE selects spectrum on the file to plot.

If the requested spectrum can not be found on LUNIT, the remaining commands for that graph are ignored and the program continues with the next graph.

The colors corresponding to LPEN are those for the AFGL Calcomp Plotter.

LSYMBL can range in absolute value from 0 to 15. The symbols corresponding to the values 1 to 15 depend upon

the plot library used and are documented in the AFGL Computer Center Memo "How to Use the Cyber Plotters." Negative values of LSYMBL supress the lines between points.

The program does not check for valid ranges of LPEN, LSYMBL and LDASH.

Cards 6a. and 6b. are read in only if LSCALE on Card 5 is 1 and then both cards are read in. If XQUAD is not zero, then the wavenumber values are scaled as follows:

V' = XOFSET + XSCALE*V + XQUAD*V**2

where V is the scaled wavenumber values.

To decrease the size of the lettering by a factor of 2, double the length of both axes and set SCALE on Card 3 to 0.5.

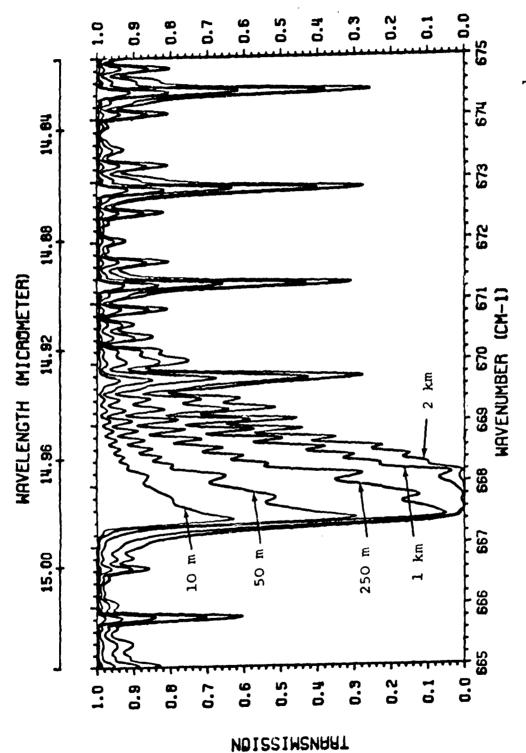
If differenced radiance is plotted on a temperature scale, then the plotted values would be the brightness temperature of the radiance difference not the difference in brightness temperatures of the two radiances.

4. SUPPORTING CALCULATIONS

One of the steps in validating the SCRIBE spectra is to compare the radiance in the 667 cm⁻¹ region and the window regions with model calculations. The region around 667 cm⁻¹ is very opaque due to absorption by the Q branch lines of the v_2 band of CO_2 . As a result, the measured brightness temperature around 667 should approximately the temperature of the air immediately in front of the instrument regardless of the instrument's orientation. The measured radiance in the window regions between 8 and 12 micrometers should be either very small in the case of upward looking spectra, or approximately equal to the ground temperature for downward looking spectra. This section will show calculations which verify and quantify these assertions.

These calculations use FASCODE to model the transmittance and radiance corresponding to conditions typical of the SCRIBE experiment. The altitude of the sensor is 30 km and the atmospheric profile used is Midlatitude Summer. The calculations have been degraded with a (sinc)² scanning function with a half width at half maximum (HWHM) of 0.053 cm⁻¹, corresponding roughly to the unapodized SCRIBE spectra.

Figure 2 shows the transmittance between 665 cm^{-1} and 675 cm^{-1} for a horizontal path (constant pressure) for ranges of 10 m, 50 m, 250 m, 1 km and 2 km. Note that for a range of 1 km the transmittance falls to below 1 percent



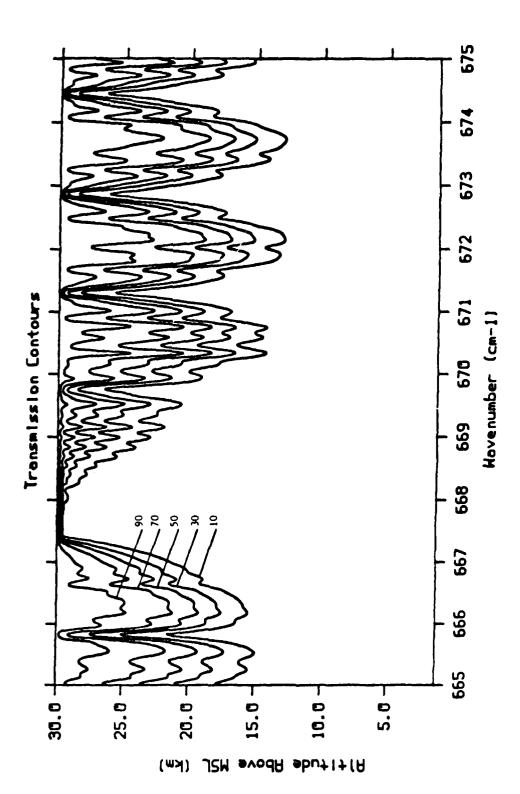
675 cm⁻¹ for a 5 Different Ranges: 10 m, 50 m, 250 m, Transmittance Between 665 and km for Calculated at 30 Horizontal Path 1 km, and 2 km. Figure 2.

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between 667.4 and 667.8 cm⁻¹. As a result, 99 percent of the radiance in this spectral region originates within the first 1 km, or in other words, the instrument can "see" no more than 1 km away. Examination of the curves for the other ranges show that 50 percent of the radiance originates within the first 50 meters, and 80 percent within the first 250 meters.

The lapse rate at 30 km for this profile is 2.6 °C/km. It can then be assumed that the air temperature 1 km in any direction from the instrument is at most 2.6 °C different from that immediately around the instrument. This maximum difference only occurs for nadir viewing geometry; for limb viewing or for horizontal viewing, the difference will be much less. The measured brightness temperature between 667.4 cm $^{-1}$ and 667.8 cm $^{-1}$ should therefore be the same (\pm about 2 OC) as the nominal air temperature at the altitude of the instrument. The calibration of the measured spectrum checked by comparing the measured brightness can be temperature around 667 cm⁻¹ with the measured air temperature, (say from a radiosonde).

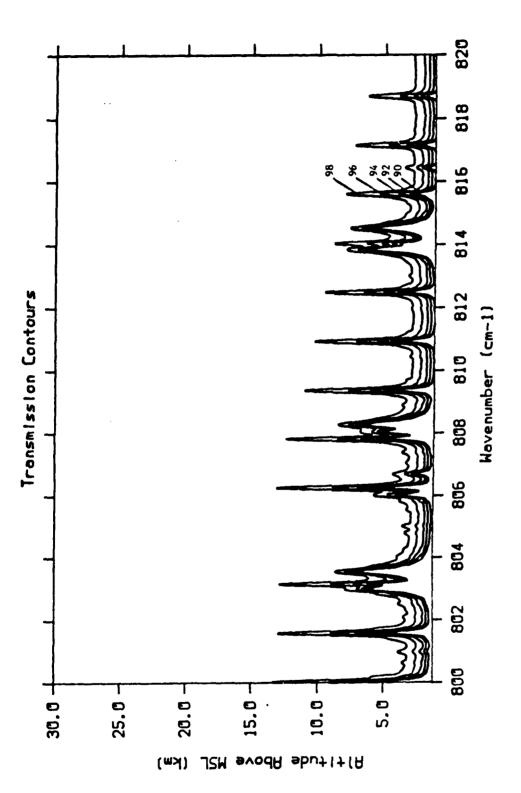
Figure 2 demonstrated that in a very opaque region of the spectrum, the measured radiance originated from the air directly in front of the instrument. This same information can be shown in a different type of graph which also shows the origin of radiance in less opaque regions or even in the window regions. Figure 3 is a contour plot with lines of constant transmittance on a graph of altitude versus



Trangmittance on a Grid of Altitude Straight Down from 30 km and Assumes the Midlatitude Summer The Calculation Models versus Wavenumber between 665 and 675 of Constant Contour Plots Sensor Looking Figure 3. Profile.

wavenumber. The figure corresponds to the case of instrument looking down from 30 km. The lines of constant transmittance indicate the altitude at which transmittance equals the indicated value. For example, following the 50 percent line, at 670 cm⁻¹ the 50 percent point is reached at 25 km while at 673.7 cm⁻¹ it is reached at 17 km. This figure shows that in the opaque region around 667 cm⁻¹, the 10 percent transmittance point occurs very close to 30 km, as expected from the previous figure. In the regions between the R branch lines, for example around 673.7 cm⁻¹, the transmittance contours penetrate much deeper into the atmosphere and indicate that the radiance originates in a broad altitude range, with 80 percent coming from between 22 and 13 km. The graph was derived from a FASCODE calculation of the transmittance for a path from 30 km to the ground using 30 layers each 1 km thick. The IMRG = 3 option was used to separately store the transmittances corresponding to the paths from 30 km to the bottom of each layer. Each one of the layer transmittances was degraded with a (sinc)² instrument function with HWHM 0.053 cm^{-1} .

A similar graph for the window region between 800 and 820 is shown in Figure 4. Between the absorption lines, the transmittance to the ground is generally 90 percent so that 10 percent of the radiance received at the instrument originates in the atmosphere. However, the 98 percent contour is at about 2 km so that 80 percent of the



Transmittance on a Grid of Altitude Straight Down from 30 km and Assumes the Midlatitude Summer The Calculation between 800 and 820 of Constant Contour Plots versus Wavenumber Sensor Looking Figure 4. Profile.

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atmospheric radiance originates within the lowest 2 km. The brightness temperature measured by the instrument will be approximately the temperature of the ground modified slightly by the lowest 2 km of the atmosphere.

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